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A Case Study of Consequences Analysis of Ammonia Transportation by Rail from Gurun to Port Klang in Malaysia Using Safti Computer Model

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Abstract

There are many ways of describing the quantitative risk assessment (QRA) methodology, but in general, the basic steps include: System Definition, Hazard Identification, Frequency Analysis, Consequence Modeling, and Risk Calculations and Assessment. The present study is aimed at the Consequence Analysis, which was an integral part in the QRA for the transportation of ammonia by rail from Gurun to Port Klang. The software package SAFETI has been used to model the resulting behavior of the released ammonia and the extent of the damage expressed in terms of distance to certain effect levels. Besides, sensitivity analysis was also carried out to identify the impacts of atmospheric conditions on ammonia gas dispersions. The results indicated an increase in the ammonia gas dispersion distances for releases at higher atmospheric temperatures of lower atmospheric humidity (e.g. for rupture case with wind speed 3m/s, at 15oC, the dispersion distance was 835.4 m, while at 35oC, it increases to 866.2 m). However, further analysis of the effects atmospheric humidity on the ammonia gas dispersions was required to determine the differences in the trend for the 25 mm and 100 mm leak cases compared to the rupture case.

Keywords: Consequence Analysis, Quantitative Risk Assessment, Rail, Transportation of Ammonia, Sensitivity Analysis.

1.0 Introduction

Rail is favored as one of the means of transport medium compared to other modes due to its ability to carry large loads. A series of road accidents in Germany in the late 1980's prompted the country to implement measures aimed at transferring certain long haul dangerous goods transport from road to rail or other means. Such effort also influenced other countries, as well as the member countries of the European Union, to review road versus rail safety issues [1]. Since then, there has been a steady increase in the use of railways as the means of transport of hazardous materials throughout the world [2]. However, as with road and other transport modes, there have been many occurrences of rail/train accidents involving releases of hazardous materials. The National Transportation Safety Board (NTSB) in the USA reported that 1986 was a tragic year for the rail transportation industry [3] because there were 17 rail accidents occurred in that year and resulted in 19 fatalities, 230 injured and over $64 million US dollars in damage. Based on the Federal Railroad Administration (FRA) 1987 - 1992 Report [4], from the year 1981 to 1991, an average of 12% of the total accidents resulted in a release of hazardous material, whilst 50% of these releases, on average resulted in evacuation of people in the surrounding areas. Although the likelihood of a hazardous material release based on the data presented above is low, the potential impact of the release to the surrounding population is significant in which one out of every two incidents involving a hazardous material release resulted in severe effects to the population.

Corresponding information provided in the annual reports of the NTSB, 1979 and 1991 [5] states that the breakdown of fatalities due to accidents by commodity type is typically as follows: Gasoline 32.5 %; LPG 21.7 %; Chlorine 9.6 %; Corrosive Liquids 9.6 %; Ammonia 6 %; Aviation Fuel 2.4 %; Compressed Gas 2.4 %; and others 15.6 %. Such information indicates that hazardous materials, like gasoline, LPG, chlorine and corrosive liquids are major causes of fatality following a rail accident releases. However, of all these hazardous materials, the risks from chlorine and ammonia releases are considered to be the worst, since both of these toxic gases are capable of spreading large distances with significant toxic gas concentrations and causing harmful effects to people.

In Malaysia, there have been no reported cases of ammonia rail accidents, due to the limited use of rail as a means to transport ammonia. The only known rail transportation mode of ammonia in Malaysia is the current transportation of anhydrous liquefied ammonia from the Petronas Fertilizers Kedah (PFK) plant in Gurun (Northern part of Peninsular Malaysia) to the Chemical Company of Malaysia (CCM) fertilizer facilities in Port Klang (South-western part of Peninsular Malaysia), with 450km length of track route. On the basis of the potential significant effects of ammonia toxic gas releases to the surrounding population and its possible outcomes as highlighted in the historical ammonia accidents [6-8], this study is devoted to the undertaking of the consequence analysis of the ammonia rail accidents for the above mentioned route. In addition, sensitivity analysis is also conducted to identify the impacts of atmospheric conditions on ammonia gas dispersions. The consequence modelling results from this study are intended to combine with the results from failure frequency analysis [9], in order to be used as an input in the QRA for the transportation of ammonia.

2.0 Literature Review

2.1 Risk of Hazardous Materials Transportation by Rail

In the transportation industry, quantitative risk assessments (QRA) have been used as a tool to help determine the safest route for the transportation of hazardous materials [10]. Among the studies carried out on hazardous materials transportation, most have been centred on materials such as chlorine, LPG and gasoline [2] [11]. The use of QRAs in the transportation industry, mainly for the transportation of hazardous materials by rail has been applied vigorously in recent years due to the concerns that most of the rail transportation routes are located close to heavily populated areas and the risks posed by the transported hazardous materials to the surrounding populations along the transportation route. Besides, case histories have also shown that the risks of hazardous materials during transport may present additional risks in addition to those associated with the inherent chemical and physical properties of the hazardous substances, mainly due to the circumstances and location of the incidents may be unpredictable [12].

In the present study, the rail transportation route of anhydrous liquefied ammonia in Malaysia, from the Petronas Fertilizers Kedah (PFK) plant in Gurun to the CCM fertilizer facilities in Port Klang, was studied due to the large amount of transported hazardous material (35,000 tons/year, 70 trips per year) and potential affected populations along the specified route (some of the residential areas and dwellings are located as close as 3 – 6m from the track).

2.2 Behavior of Ammonia Upon Release

Ammonia is an important chemical for use primarily in the manufacturing of fertilizers and also as the starting material for the manufacture of a great variety of chemicals. It is a colorless gas, lighter than air and has a very pungent odor. It can be liquefied at atmospheric pressure by reducing the temperature to -330C and usually stored and transported as a pressurized and/or refrigerated liquid. Typically, ammonia releases into the environment can be classified into three types of behaviours under operating conditions such as [13]: Pressurized Liquid above its Boiling Point (known as superheated liquid), Pressurized Liquid below or at its Boiling Point, and Pressurized Gas above its Boiling Point. In this study, the behaviour of ammonia following a rail transport accident is expected to be the superheat liquid, based on the case study rail car storage temperature and pressure.

Due to the stored heat energy of the liquid ammonia (also known as sensible heat), some of the liquid ammonia will flash to vapour following an incident and upon a release. However, depending on the type and location of the leak, flashing may result in two phase release, which will produce a finely dispersed liquid or an aerosol that lead to more vapour formation when it vaporizes owing to heat transfer with the entrained air and also due to endothermic reactions with moist air. Thus, the fraction of liquid ammonia that will flash, calculated from the thermodynamic equation refer to equation 1 below], will produce an underestimate of the amount of ammonia that would actually flash to vapor and disperse.

$$\mathbf{f = Cp\ (Ts - Tb) / hfg} \quad \text{(Equation 1) [14]}$$

Where:

- f = fraction of liquid
- Ts = ammonia storage temperature (K)
- Tb = boiling temperature of ammonia at ambient temperature (K)
- Cp = specific heat at constant pressure of the liquid ammonia (J/kg/K)
- hfg = heat of vaporisation of ammonia (J/kg)

Experiments carried out, by Johnson (1991) shows that little aerosol formation occurs at low levels of superheat, (Ts – Tb) [14]. As the level of superheat increases, the liquid discharged starts to break up and changes from a continuous stream of liquid to stream of liquid droplets, the higher the superheated level, the higher the extent of the aerosol formation.

In this study, an assumption is made that all the liquid ammonia released will flash to form an aerosol and vapour mixture, which is considered to be the worst case consequence possible following an accidental release of ammonia.

2.3 SAFETI Software Description

Consequence modelling is an essential step of the overall QRA process and is used to predict the behaviour of hazardous incidents. There are many software models available to calculate the consequences from an incident; most of these models estimate the quantities of material that will be released, the resulting behaviour of the material released and the extent of damage expressed in terms of distance to certain effect levels. In this study, the Software for the Assessment of Flammable, Explosive and Toxic Impacts (SAFETI) developed by Det Norske Veritas [15] has been used to analyse the physical effects of ammonia gas releases following a leak or rupture from the rail car tank, and the subsequent damage posed by the release to the surrounding people.

There are three basic models provided in SAFETI to determine the release characteristics (an instantaneous release, a release through a sharp edged hole, and a release through a pipe). Used alone or in combination these models can determine the release characteristics of holes in tanks, pipe leaks, relief valve and bursting disc releases, flange leaks, tank ruptures and so on. For the dispersion modeling of a cloud at all points of interest, SAFETI uses the self-embodied Unified Dispersion Model (UDM), which uses a number of models (i.e. the turbulent jet phase, dense turbulent plume phase, slumping dense and passive dispersion phase) with each applicable in its own range and match the cloud parameters as the program changes between models. The UDM model within the SAFETI software package have been subject to detailed verification and validation against field experiments as well as other models by Witlox and Holt [16 – 20]. Turbulent jet phase is the first stage that a release may pass through, where the actual conditions of release (velocity or expansion energy) determine how rapidly air is entrained. Dense turbulent plume phase is the second stage, which is a mixture of the initial turbulence stage and dense cloud behaviour. During this phase the release is still entraining air at a rate determined by the initial turbulence but it has started to spread laterally over the ground due to its greater density than the ambient air. Eventually the cloud begins to behave as a purely dense cloud and in this third stage (slumping dense) the rate of entrainment as well as the spreading is purely determined by dense cloud behavior. The fourth stage is when the ambient atmospheric turbulence is the dominant influence on entrainment and spreading and the behavior is that of a passive release.

3.0 Methodology

The consequence modeling begins with the release of transported ammonia from the rail car tank, either due to the car tank failure from accident forces or due to the relief valve being opened, owing to high pressures caused by an external fire. The following is a simple three-step procedure adopted in this study based on the approach identified by Rhyne [5] and is further illustrated in Figure 1:

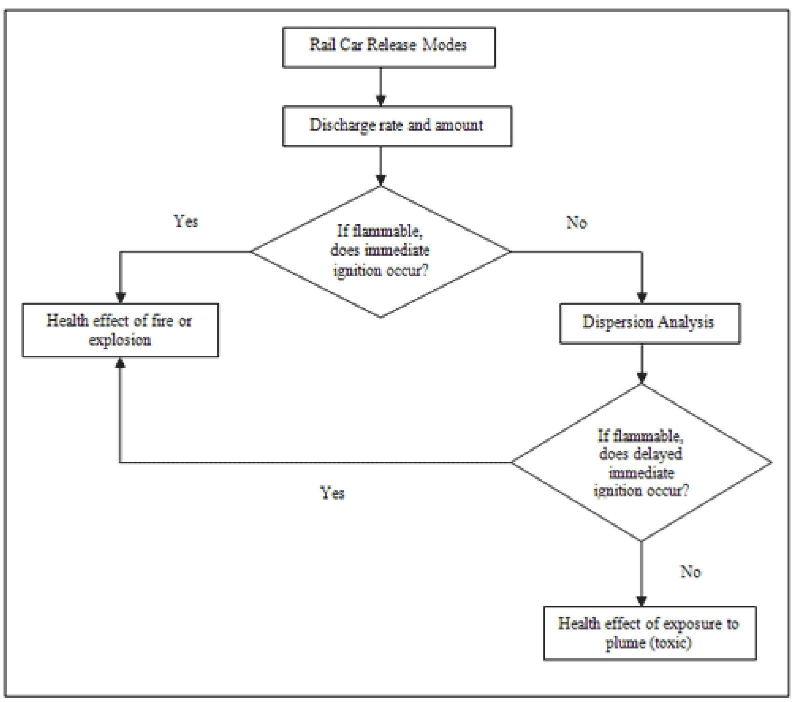

Figure 1. Consequence Modeling Procedure Adopted

1. Definition of the source term, which deals with the release mode and the amount released
2. Exposure assessment, which deals with the extent of the exposure to people due to the source term; and
3. The assessment of health effect of people exposed to the source term

3.1 Release Modes

In this study, the release modes have been determined (from failure frequency analysis) as the types of accident events, which could occur as a result of a rail accident (train collisions or derailments). The accident events considered are related to railcar tank crush, puncture, and impact releases on the tank head, tank shell, liquid valve, gas valve, valve dome and man way of the tank [9].

Windspeed at 1m height from ground level	1.5 m/s, 3.0 m/s, 5.0 m/s and 9.0 m/s
Wind direction	North, North-East, East, South-East, South-West, West, North-West
Pasquill stability	B, D and F
Average temperature	27°C (300 K)
Relative humidity	82%

Table 1. Selected Meteorological Conditions

	Percentage of Occurrence of Each Combination of Windspeed/Atmospheric Stability at a Height of 1m				
Direction	3.0 m/s B	1.5 m/s D	5.0 m/s D	9.0 m/s D	1.5 m/s F
N	3.392	0.975	2.104	0.145	9.617
NE	1.490	0.846	3.544	0.054	6.077
E	1.877	0.590	2.039	0.060	5.431
SE	2.097	0.446	0.797	0.066	2.661
S	5.153	0.389	1.132	0.200	3.225
SW	7.256	0.363	7.143	0.202	2.448
W	5.466	0.335	4.103	0.228	2.535
NW	4.218	0.655	0.839	0.149	6.661

Table 2. Weather Probabilities

Meteorological data, such as wind speed and direction, Pasquill stability, temperature, and relative humidity form part of the initial conditions of the releases, and thus considered as part of the definition of the source term. Pasquill stability is usually measured using the Pasquill-Gifford Scale, ranging from A to F, with A being most unstable atmospheric condition and F being most stable atmospheric condition [21]. Table 1 shows the meteorological conditions while Table 2 presents the weather probabilities adopted in this consequence analysis, which are based on similar meteorological conditions that used in the analysis carried out by the Liberty Risk Services Malaysia (LRSM) [13]. Noted that the weather probabilities are averaged for both night and day over a 24-hour period assuming a 50:50 split between night and day. Sensitivity analysis was also carried out to identify the impacts of atmospheric conditions on ammonia gas dispersions, where a temperature range between 150C and 350C, and a relative humidity range between 60% and 90% were analyzed.

3.2 Discharge Modeling

The aim of the discharge modeling is to go from the initial conditions to predict the final state of the release as the material emerges into the atmosphere following an accidental release. For all the case study scenarios modeled (same as that used in the previous failure frequency analysis [9]), the program predicts the condition of ammonia upon discharge until the release has expanded down to atmosphere pressure. The initial conditions that have been set as inputs within the program are as follow:

Inventory of release	=	20000 kg (i.e. rail car storage capacity)
Storage temperature	=	300 K (i.e. above the boiling point of ammonia)
Leak source	=	modeled as a vapor release (i.e. behavior upon release)
Surface Type	=	Dry Soil (i.e. ground surface conditions following a release)
Surface Roughness	=	0.17 (i.e. rougness of surface following a release with default value of 0.17 representing residential areas, industrial sites, woods, etc.)
Atmospheric Pressure	=	101.3 kN/m^2
Atmospheric Temperature	=	300 K

Three different hole sizes, i.e. 25mm, 100mm and tank ruptures have been assumed to represent the distributions of possible release size [9]. The 25mm and 100mm hole sizes are modeled as continuous releases, while the rupture scenario is considered as instantaneous releases. The flow rates calculated within the program represent constant release rates, which are conservative, compared to reality, in which the flow rate will decrease with decreasing pressure and inventory.

3.3 Dispersion Modeling

In general, there are four distinct stages that an ammonia release may go through upon a release (i.e. turbulent jet, dense turbulent plume phase, slumping dense plume phase, and passive dispersion phase). Each of these stages is modeled in SAFETI through smoothly matched models using a simple form of concentration profile to cover all stages for a release [22]. The dispersions of ammonia are modeled based on each case study scenario, adopted in the failure frequency analysis [9].

3.4 Toxic Effect Modeling

Ammonia is difficult to ignite in the open air as its flame is unstable and cannot propagate itself. Though explosions can occur in flammable mixtures in vessels or enclosed spaces, the ignition is difficult and the possibility of an explosion in the open air is generally discounted. Therefore, ammonia is not considered a significant fire and/or explosion hazard. In this study, emphasis is given on the toxic effects of ammonia. The toxic effect consequence models within SAFETI use the output from the dispersion models to calculate the effects on people (or effect zone), given the specified release and weather conditions. Toxic consequences are expressed as one set of results, which give the variation in fatality risk with distance from the release point. In this study, the Immediately Dangerous to Life and Health (IDLH) exposure limits and the “Probit Equation” (refer equation 2 below), incorporated within SAFETI program are used to determine the toxic effects of ammonia.

$$\mathbf{Y = k1 + k2 \ln V} \quad \text{(Equation 2) [21]}$$

Where:

- Y = the probit variable
- k1 and k2 = probit parameters
- V = causative variable

4.0 Results and Discussions

4.1 Toxic Effect of Ammonia Upon Release

Probit function is a normally distributed function with a mean of 5.0 and a variance of 1.0. A probit of 5.0 corresponds to 50% fatalities, 3.36 to 5% fatalities and 6.64 to 95% fatalities. The corresponding probit numbers for all the scenarios modeled in the case study, calculated within the SAFETI program, are shown from Figure 2 to Figure 7.

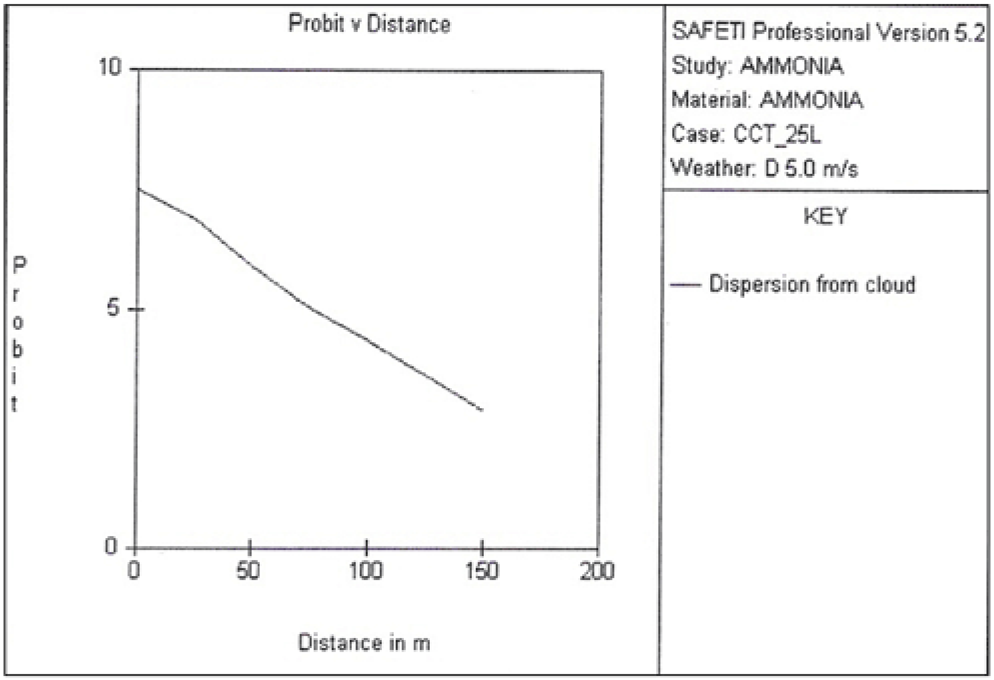

Figure 2. Collision Crushing Tank Scenario - 25mm Leak

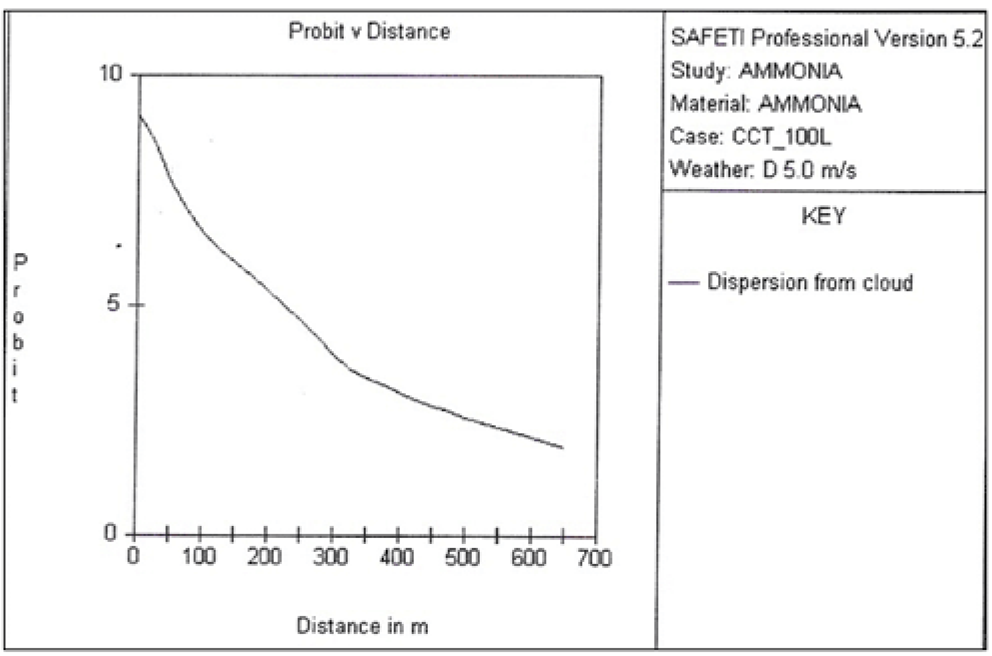

Figure 3. Collision Crushing Tank Scenario - 100mm Leak

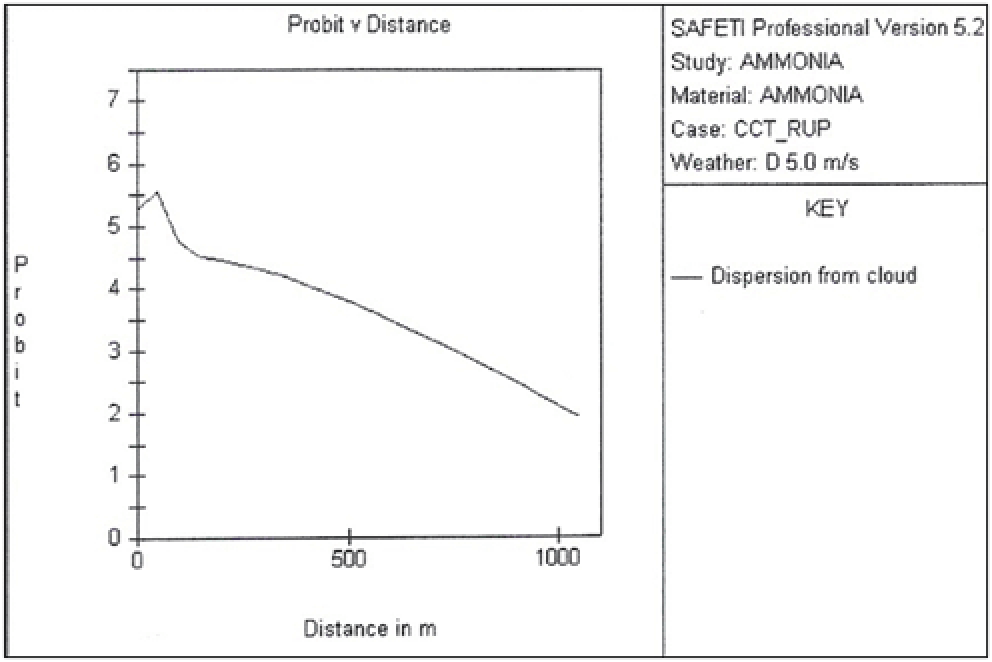

Figure 4. Collision Crushing Tank Scenario - Rupture

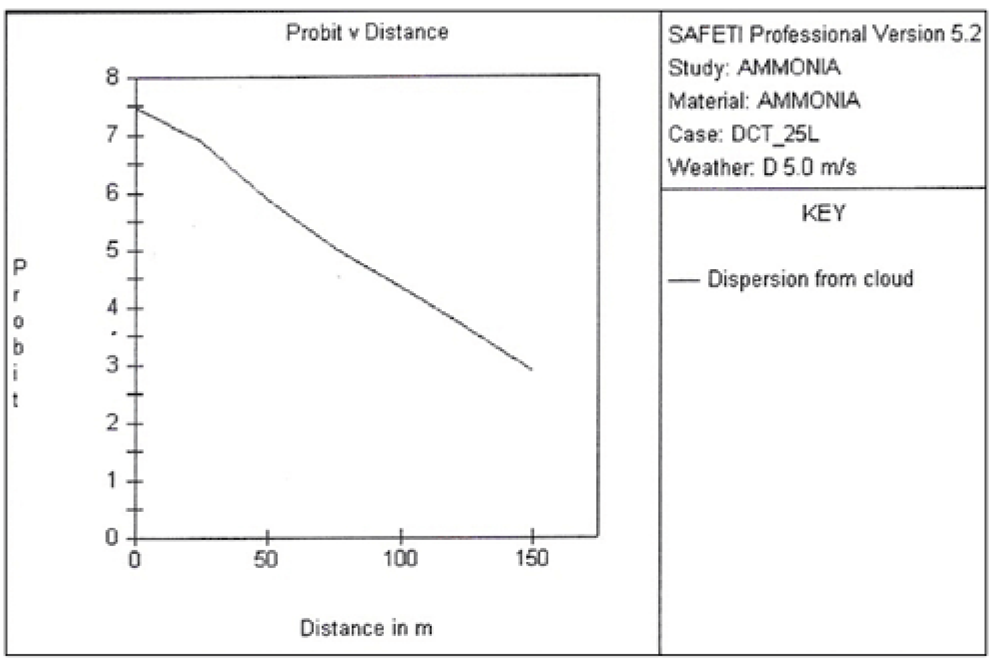

Figure 5. Detrailment Crushing Tank Scenario - 25mm Leak

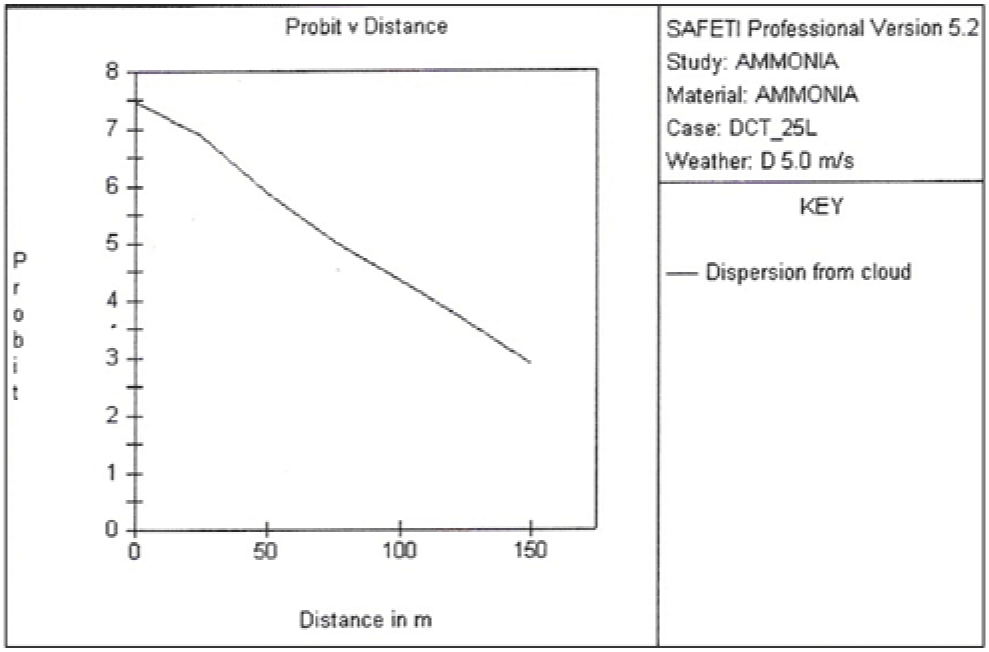

Figure 6. Derailment Crushing Tank Scenario - 100mm Leak

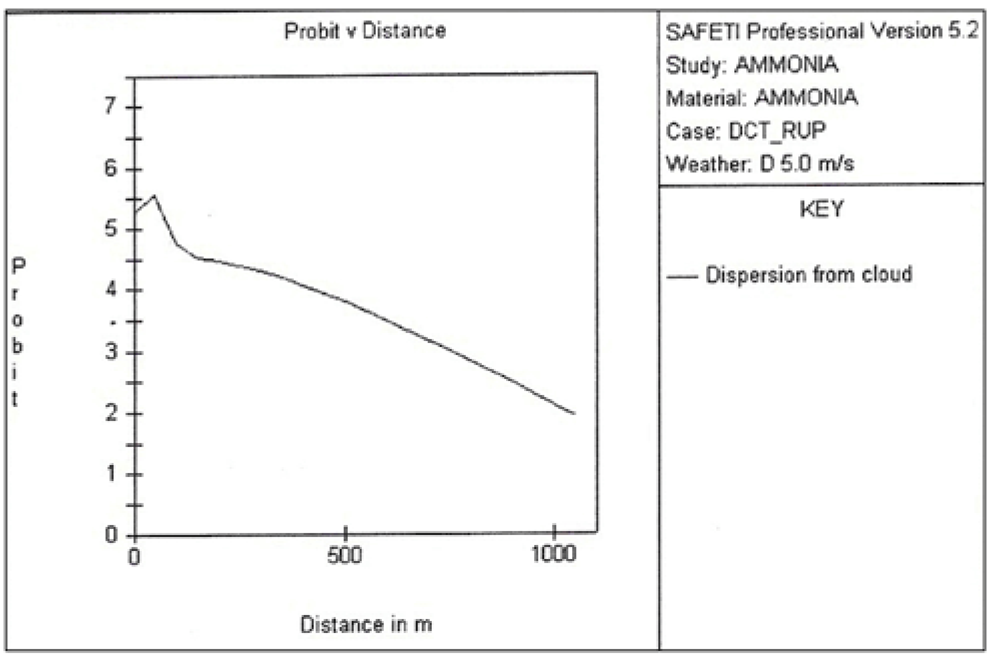

Figure 7. Derailment Crushing Tank Scenario – Rupture

4.2 Effects of Atmospheric Conditions on Ammonia Dispersions

	Distances from the Centre of the Railway Track to the IDLH Exposure Limits for Ammonia Gas Releases (meter)					
	Windspeed 3 m/s, PasquillStability B			Windspeed 5 m/s, Pasquill Stability D		
Atmospheric Temperature (C°)	CIH 25mm leak case	CIH 100mm leak case	CIH rupture case	CIH 25mm leak case	CIH 100mm leak case	CIH rupture case
15	102.9	408.6	835.4	171.4	713.2	1972.0
20	103.6	412.8	840.4	172.3	721.8	1989.1
25	104.2	420.4	852.0	174.2	729.6	2005.8
30	105.7	432.5	859.2	179.7	743.2	2022.6
35	106.1	437.5	866.2	181.6	749.0	2039.2

Table 3. Effects of Temperature on Ammonia Gas Dispersions

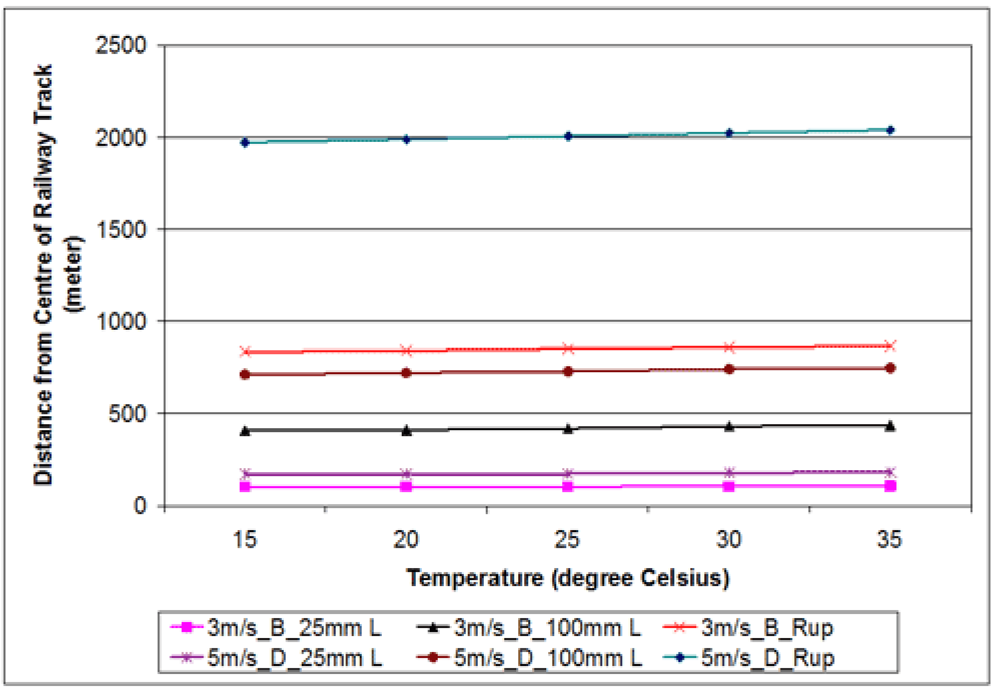

Figure 8. Effects of Temperature on Ammonia Gas Dispersions

	Distances from the Centre of the Railway Track to the IDLH Exposure Limits for Ammonia Gas Releases (meter)					
	Windspeed 3 m/s, PasquillStability B			Windspeed 5 m/s, Pasquill Stability D		
Relative Humidity (%)	CIH 25mm leak case	CIH 100mm leak case	CIH rupture case	CIH 25mm leak case	CIH 100mm leak case	CIH rupture case
60	105.3	448.3	831.1	180.0	749.4	1998.2
70	105.1	442.9	844.4	179.7	749.0	2004.9
80	104.8	432.0	854.7	175.2	731.1	2012.1
90	104.5	423.0	854.8	174.6	732.8	2012.3
95	104.2	429.7	859.9	174.5	726.6	2070.2

Table 4. Effects of Humidity on Ammonia Gas Dispersions

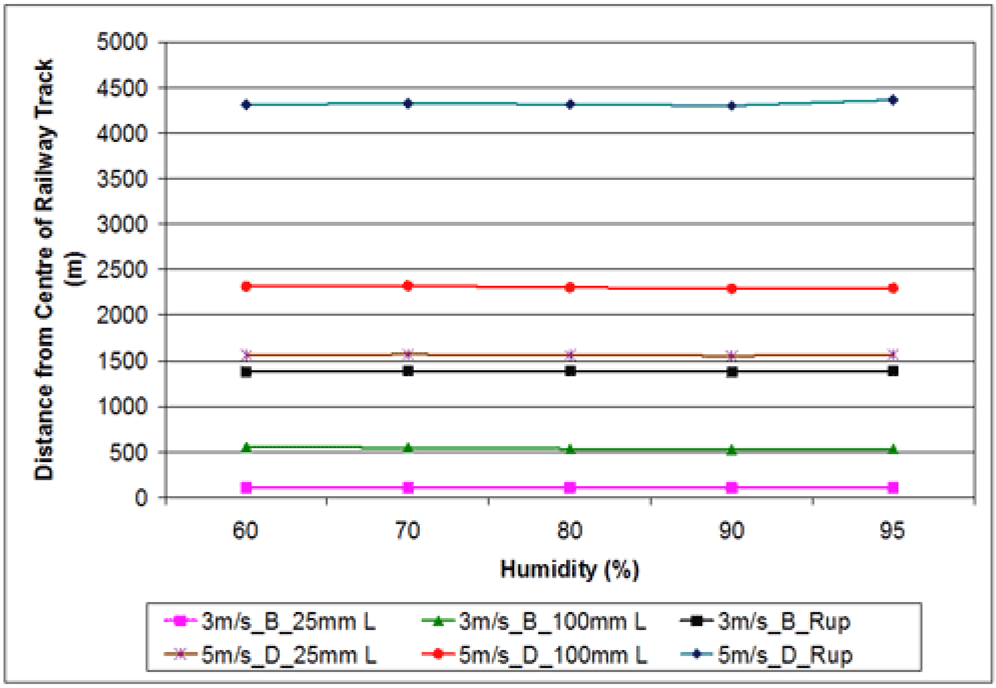

Figure 9. Effects of Humidity on Ammonia Gas Dispersions

Table 3 and Figure 8 show the effects of temperature on the dispersions of ammonia for a temperature range between 150C and 350C whilst Table 4 and Figure 9 show the effects of humidity on the gas dispersion modeling of ammonia releases for a humidity range of between 60% and 95%. It should be noted that the sensitivity analysis was carried out using the following three failure scenarios as representative cases with two weather categories; wind speeds of 30 m/s and 5.0 m/s with Pasquill stability class, B and D, respectively:

- Collision Impact Force Fails Tank Head (CIH) – 25mm hole leak
- Collision Impact Force Fails Tank Head (CIH) – 100mm hole leak
- Collision Impact Force Fails Tank Head (CIH) – tank rupture

The results from Table 3 shows that the ammonia gas dispersion distances from the centre of the railway track to its IDLH exposure limits (i.e. concentration of 500ppm) increases with increasing atmospheric temperature. The change in the gas dispersion distances from the centre of the track varies from about 3 – 10m for the 25mm leak case, 29 – 36m for the 100mm leak case and 31 – 67m for the rupture case, depending on the wind speed and atmospheric stability. The results indicate that ammonia gases released at higher atmospheric temperatures will disperse larger distances with significant levels of toxic concentrations. However, the effects of temperature on the ammonia gas dispersion are only minimal for the temperature range considered in the analysis, with an increase in the dispersion distances by about 3 – 7% only for the scenarios analyzed. Figure 8 also indicates that the ammonia gas dispersion distances are greater for wind speeds of 5 m/s at Pasquill Stability D compared to wind speeds of 3 m/s at Pasquill Stability B, due to the higher wind speed and more stable atmospheric conditions associated with the former, resulting in less mixing and entrainment of air during the gas dispersion, hence the gas is dispersed greater distances with significant levels of toxic concentration before being dilution to concentrations not harmful to people.

Table 4 shows that the ammonia gas dispersion distances from the centre of the railway track to its IDLH exposure limits (i.e. concentration of 500ppm) decreases with increasing atmospheric humidity for the 25mm and 100mm leak scenarios but increases with increasing atmospheric humidity for the rupture scenario. The change in the gas dispersion distances from the centre of the track varies from about 1 – 6m for the 25mm leak case, 19 – 23m for the 100mm leak case and 29 – 72m for the rupture case, depending on the wind speed and atmospheric stability. Figure 9 shows that the effects of humidity on the ammonia dispersion results are only minimal for the humidity range considered in the analysis, with a difference in the dispersion distances by about 0.5 – 6% for the scenarios analyzed. Figure 9 also indicates that the ammonia gas dispersion distances is greater for wind speeds of 5 m/s at Pasquill Stability D compared to wind speeds of 3 m/s at Pasquill Stability B. Thus, the gas is dispersed greater distances before being dilution to concentrations not harmful to people.

5.0 Conclusions

Based on the IDLH exposure limits for ammonia (i.e. 500ppm) and the toxic equations incorporated in the SAFETI software packages, the consequence modeling dispersion results show that ammonia gases disperses fairly large distances with significant levels of toxic concentrations before the process of dilution to a less harmful concentration. Thus, most of the surrounding populations along the railway track will be subjected to a high exposure of toxicant following the releases of ammonia due to the rail accident (collision or derailment). It is suggested that the clearance zone for residential areas and industries specified by the Malaysian National Railway, which is 15m from the track, should be reviewed in order to take into consideration the consequences resulting from the transported materials. Besides, the results also demonstrate the need for the proper planning and operations on the transportation of the ammonia cargoes from the PFK plan to the storage facilities in Port Klang. Priority should be given for moving the ammonia transported train through populated areas as quickly as possible. This will help to minimize the exposure to these people since the risks from the ammonia cargoes are only present when the transport vehicle passes through the populated area and at other times the risks are absent, since the hazards are not present.

Sensitivity analysis carried out in the study identified the impacts of atmospheric conditions on ammonia gas dispersions. The consequence modeling results indicates and increases in the ammonia gas dispersion distances for releases at higher atmospheric temperatures or lower atmospheric humidity. However, further analysis of the effects atmospheric humidity in the ammonia gas dispersions is required to determine the differences in the trend for the 25mm and 100mm leak cases compared to the rupture case. The influence of the atmospheric conditions on the ammonia gas dispersion results are however, only minimal for the range considered in the analysis. Nonetheless, the effects are expected to be more significant in surrounding where the differences in temperature and/or humidity are more extreme; i.e. in countries with more diverse change in atmospheric conditions than in Malaysia.

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